Dimethyl ether 115-10-6 | DTXSID8026937

Model Performance

le .	
Model Data	
Model	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 1820 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.45e-01

Confidence level: 6.78e-01

Nearest Neighbors from the Training Set

Image not found

1-Tetradecanol Measured: 4450 Predicted: 1.08e-04

Image not found

1,2-Dichloroethylene Measured: 1490 Predicted: 120

Image not found

1,1,1,3,3-Pentafluoropropane

Measured: 300 Predicted: 1780

Image not found

Bromoacetone Measured: 605 Predicted: 38.1

Image not found

2-Mercaptoethanol Measured: 538 Predicted: 7.89e-01